Failure of Valence Bond Theory / Why need of Hybridisation?

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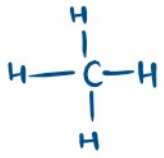
Previous concept : VBT

How CH_4 molecule formed ? (According to VBT)

We have to make four bonds with C



Electronic Configuration of Carbon:

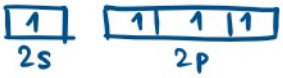
$_6C \rightarrow 1s^2 2s^2 2p^2$

Two unpaired electrons

According to VBT, unpaired electrons forms bond.

To form 4 unpaired electron, Carbon goes to

1st excited state :



Four unpaired electrons available for 4 bonds formation.

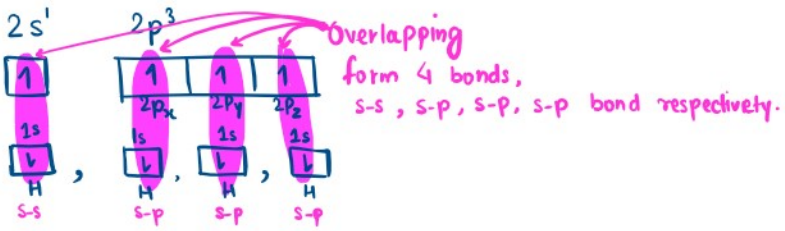
Electronic configuration of Hydrogen = $1s^1$

1 Unpaired electron = 1 bond formation.

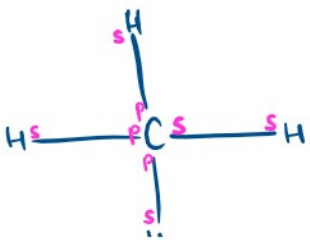
According to VBT, electrons of two atoms, with opposite spin overlap to form bond.

1st excited state of Carbon : $2s^1$ $2p^3$

Four Hydrogen :



4 bonds forms: 1 bond is s-s type and other three bonds are s-p type.

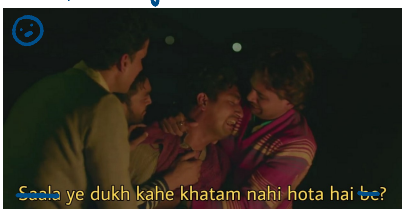


According to VBT,
Bond types are different due to formation of different orbitals overlapping.

According to experiment,
All 4 bonds of Methane are equivalent in all respect.
Bond length same.
Bond Energy same.

This mark the failure of VBT and explain later by hybridization concept.

Fun Fact : VBT is failed and replaced by Hybridization.
Hybridization theory is failed later and replace by VSEPR



Notes by : Ruhul Amin Alig

Hybridisation -Basics and Introduction

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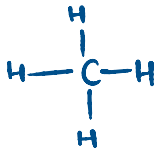
Previous concept : VBT

How CH_4 molecule formed ? (According to Hybridization)

We have to make four bonds with C



Electronic Configuration of Carbon:

$_6C \rightarrow 1s^2 2s^2 2p^2$

Two unpaired electrons

According to VBT, unpaired electrons forms bond.

To form 4 unpaired electron, Carbon goes to

1st excited state :

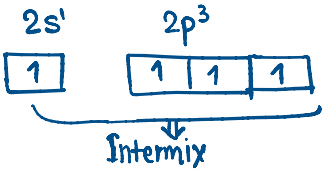
four unpaired electrons available for 4 bonds formation.

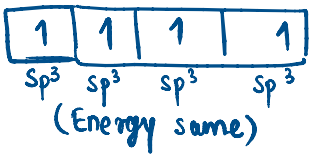
According to Hybridization ,

- Atomic orbitals of same or nearly same energy intermix to give new orbitals of exactly same energy.
- Number of previous orbitals = Number of new orbitals form.

1st exiceted state of Carbon have 4 e^- in 2s & 2p orbitals with total 4 orbitals. As orbit is same i.e 2, energy is nearly same. These orbitals intermix to form 4 new orbitals of exactly same energy (i.e sp^3 orbitals each).

1st excited state of Carbon :





(Hybrid orbitals)

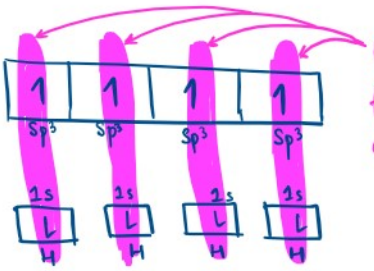
Energy is same for all hybridized orbitals BUT
In each hybridized orbital of C, which is sp^3, p character is 3 times more than s character.
This is because 3 p-orbitals contribute and only 1 orbital contribute in forming this hybridization

Electronic configuration of Hydrogen = 1s¹

1 Unpaired electron = 1 bond formation.

According to VBT, electrons of two atoms, with opposite spin overlap to form bond.

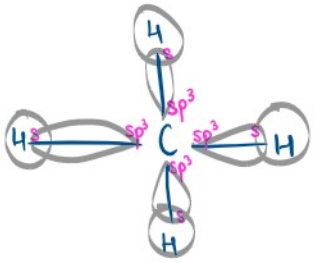
Hybridized orbitals of Carbon in 1st excited state:



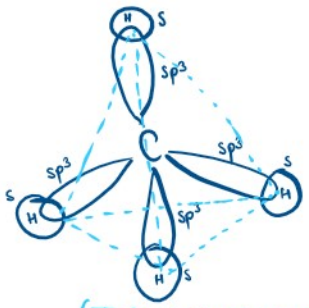
Overlapping form 4 bonds all of sp^3-s type.

Four Hydrogen

4 bonds forms: All of sp^3-s type.



All four orbitals repel each other and shape into minimum energy structure.



(Tetrahedral geometry of Methane)

Thus hybridization is responsible for geometry of a compound.

Hybridisation Theory - Key Points

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Definition:

- Intermixing of atomic orbitals of equal or nearly equal energy to form orbitals of exactly same energy or forms identical orbitals.

Which orbitals can have hybridization?

- Half filled orbital,

  Empty orbital (Vacent orbital)

  Fully filled orbitals

- Vacent or empty orbital hybridization is seen in Co-ordinate bonds.
- Coordinate bond: One atom give two electrons and another atom takes two electron to its vacent orbital.
- lone pair give fully filled orbital hybridization.

Number of hybrid orbital

The number of hybrid orbital is equal to intermixing orbitals.

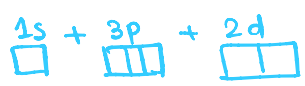
Hybridization cause by

Concept of hybridization is for sigma and lone pair.

No pie bond form hybridization

Naming of hybrid orbital

Name of hybrid orbital is named after parent orbitals.



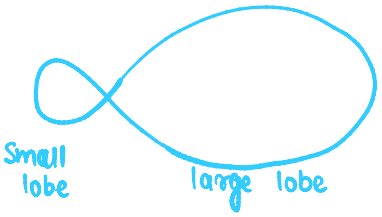
etc...

Shape of hybrid orbitals :

Hybrid orbital have its own shape of each.

Common shape of all hybrid orbital :

Sp, Sp^2, Sp^3 ⟹



Small lobe is generally not represent

Orientation

The hybrid orbitals oriented such that the repulsion is less

less repulsion, more stable.

This gives geometry to a compound.

Types of Hybridisation / Geometry / Examples

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Sp hybridization

1s + 1p = sp sp

linear.
Sp

Geometry : linear

Example : BeF_2

F — Be — F

$_4Be : 1s^2 2s^2$

1↓

•Excited:

$_4Be : 1s^2 2s^1 2p^1$

1 | 1

Hybridization

1 | 1

Sp Sp

$_9F : 1s^2 2s^2 2p^5$

1↓ | 1↓ 1↓ | 1

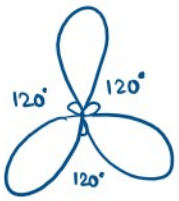
•1 unpaired electron in p-orbital

1st Bond form between sp-hybridized orbital of Berillium with p- orbital of Fluorine.

Similary second bond form.

Sp^2 Hybridization

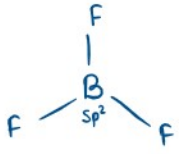
1s + 2p = sp^2 sp^2 sp^2



Trigonal planar
sp^2

Geometry: Trigonal planar.

Example : BF_3



$_5B \rightarrow 1s^2 2s^2 2p^1$

1↓ | 1 | |

1st excited state :

$2s^1 2p^2$

1 | 1 | 1 |

Hybridization

sp^2 sp^2 sp^2

1 | 1 | 1

$_9F \rightarrow 1s^2 2s^2 2p^5$

1↓ 1↓ | 1 |

1 unpaired e⁻ available for bonding

3 unpaired e⁻ for bonding

1st hybridised bond form between sp^2 of boron and P of Fluorine 1.

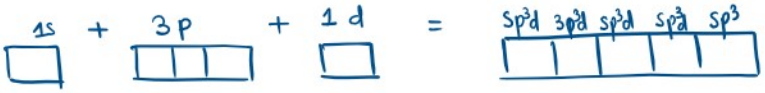
2nd " " " " " " " " " " " " 2.
3rd " " " " " " " " " " " " 3.

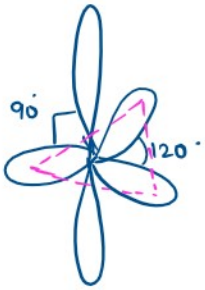
Sp^3 hybridization

Tetrahedral Geometry

Example: CH_4

Sp^3d hybridization

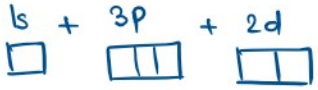




Trigonal bipyramidal

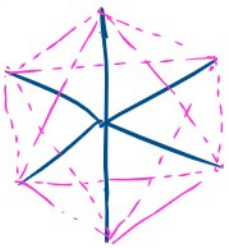
Example: PCl_5

Sp^3d^2 hybridization



= 6 orbital with sp^3d^2 each.

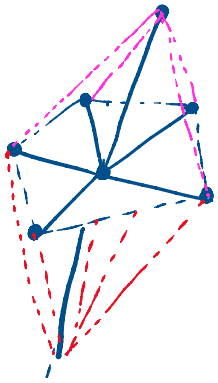
Geometry: Octahedral.



Sp^3d^3 hybridization

7 hybrid orbital.

Geometry : Pentagonal bipyramidal



How to find hybridisation ?

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Question: Find the hybridisation of Sulphur in SO_4^{2-} (sulphate ion) ?

There are two ways of finding hybridisation :

① By formula

② By structure (ie single bond + lone pair)

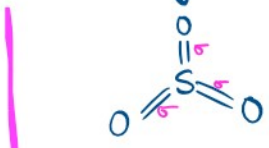
Finding hybridization by structure :

Z = no. of σ bond + lone pair of Central atom.

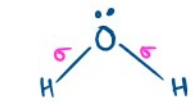
Z	Hybridization
2	Sp
3	Sp^2
4	Sp^3
5	Sp^3d
6	Sp^3d^2

• σ bond is single bond.

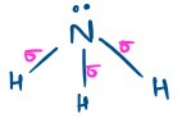
Example :



Z = 1+1+1
= 3
∴ Sp^2

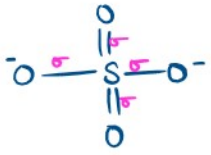


Z = 1+1+1
= 3
∴ Sp^2



Z = 1+1+1 + 1
= 4
∴ Sp^3

Sulphure in sulphate ion



Z = 1+1+1+1
= 4
∴ Sp^3

Finding hybridization by formula :

$$Z = \frac{1}{2}(\text{no. of valence } e^- \text{ on central atom} + \text{negative charge} - \text{positive atom} + \text{number of monovalent atoms (H, F, Cl, Br, I)})$$